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# PARACHORS OF CYCLIC ESTERS OF CARBONIC, SULFUROUS, AND PHOSPHOROUS ACIDS

B. A. Arbuzov and V. S. Vinogradova
Sci-Res Chem Inst imeni A. M. Butlerov,
Kazan State U imeni V. I. Ul'yanov-Lenin
Submitted 28 March 1949

/The physical constants of the phosphorous acid esters listed below are of interest, because compounds of this general type may exhibit specific toxic properties or serve as intermediates in the preparation of toxic compounds. This refers to a potentiality rather than an actual intention on the part of the Russian investigators. No actual intention to conduct work with the view of synthesizing toxic compounds has been mentioned in the article./

In order to determine the possibility of applying the group-correction method used in the case of five- and six-membered rings of carbocyclic compounds to the calculation of the parachors of heterocyclic compounds as well, the parachors of a number of cyclic esters of carbonic, sulfurous, and phosphorous acids were computed.

The group method (in which the parachors of individual groups of a ring are simply added) was found to be completely applicable for five- and six-membered heterocyclic rings containing an atom of oxygen, oxygen and sulfur, or oxygen and phosphorus in the ring.

The group values were determined for the parachors of the following groups contained in the rings:

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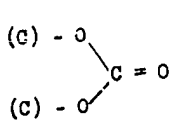
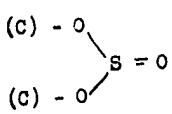
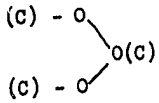
Cyclic Esters of Phosphorous Acid







The author and his co-worker determined the parachors of four esters which V. M. Zoroastrova had previously (A. Ye. Arbuzov, V. M. Zoroastrova, and N. I. Rizpolozhenskiy, IAN SSSR, OKN, 208, 1948 /see 00-W-4400/49/) synthesized through the action of alcohols on acid in the presence of pyridine or dimethylaniline. Her data for their constants are reproduced in the following table along with Arbuzov and Vinogradova's data on their parachors determined in this instance.

/See table on following page/



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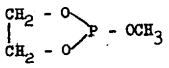
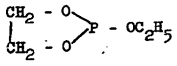
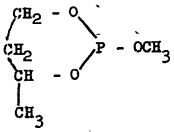
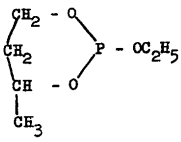
| Substance | Bp | $d_0^{20}$ | $n_D^{20}$ | $\gamma^{20}$ | Standard Ideal Value | Correction for Expansion | Parachor (computed) | Parachor (found) | Deviation in % | Corrections |
|---|---|---|---|---|---|---|---|---|---|---|
|  | 55-56°/ 23 mm | 1.2200 | 1.4460 | 35.40 | 243.5 | 0.6 | 244.1 | 244.06 | 0 | -5.4 for a five-membered ring |
|  | 51.5-52°/ 15 mm | 1.1357 | 1.4398 | 38.47 | 281.5 | 0.7 | 282.2 | 281.4 | -0.3 | -5.4<br>-1.4 beta-correction for an ester chain |
|  | 62°/13 mm | 1.1102 | 1.4420 | 31.22 | 317.3 | 0.9 | 318.2 | 319.6 | +0.5 | -10.7 for a six-membered ring<br>-3.2 for a side chain<br>-1.7 methylene-correction |
|  | 63-64°/ 8 mm | 1.0709 | 1.4405 | 29.60 | 355.3 | 1.2 | 356.5 | 353.4 | -0.8 | -10.7<br>- 3.2<br>- 1.7<br>- 1.4 |

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